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Use of Multi-Criteria Decision Making for Selecting Chemical Agent Simulants for Testing

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Working Group 2 – Nuclear, Biological, and Chemical Defense

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EDGEWOOD CHEMICAL BIOLOGICAL CENTER

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Outline

- **Background**
- **Process and Methodology**
- **Initial Applications**
- **Future Plans and Acknowledgments**

Background

- **Project initiated in 2006 as part of DTRA JSTO Tech Base T&E program (CA06TAS438)**
  - Initial task was two-fold
    - Develop a standardized process for simulant selection
    - Implement process to conduct initial simulant selection for Protection applications, and conduct testing to verify results
  - Three-year effort
- **Multi-organizational, collaborative approach for initial planning and process development**
- **Dugway Proving Ground (DPG) and the Edgewood Chemical Biological Center (ECBC) led the implementation phase**

Background

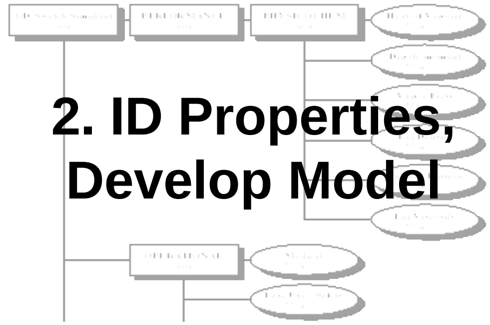
- **Year One:**
  - Reviewed previous simulant selection efforts
  - Developed initial process and vetted through community
  - Developed plan and scope for initial simulant selection
- **Year Two:**
  - Conducted simulant selection process for HD and GD, then for GB and VX
  - Conducted initial “usability” testing on output from first downselect
- **Year Three:**
  - DPG is currently conducting verification testing on simulants which resulted from second downselect

Process Overview

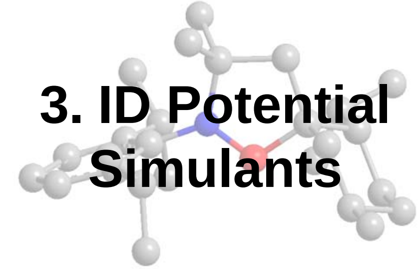
- **ECBC Decision Analysis Team (DAT) led the process development**
- **Process leveraged previous simulant selection efforts**
  - International Task Force 8 (ITF 8), late 1980's / early 1990's (Stuempfle, et. al.)
  - Chemical Biological Threat Agent Simulant Plan of Action, 2002 (Stuebing, et. al.)
  - Agent to Simulant Selection Methodology for Artemis (Chemical Agent Standoff Detection System), 2003 (Garrett, et. al.)

Process Overview

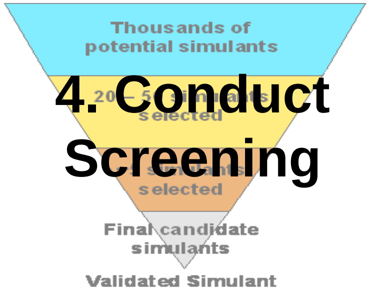
1. Frame Problem



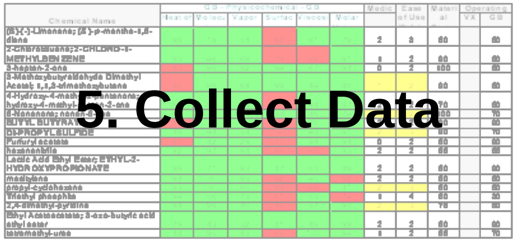
2. ID Properties, Develop Model



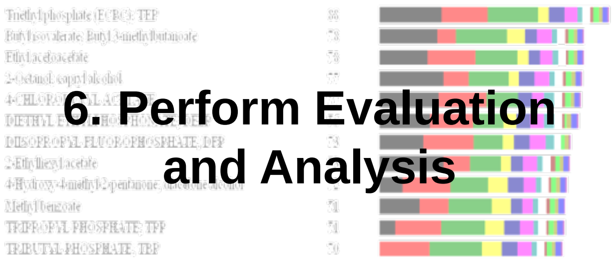
3. ID Potential Simulants



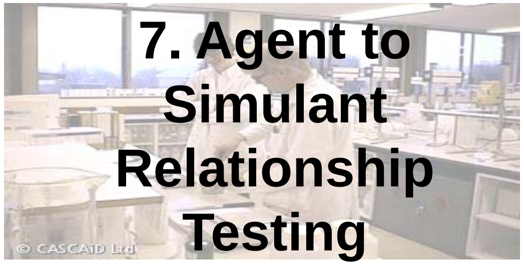
4. Conduct Screening



5. Collect Data



6. Perform Evaluation and Analysis



7. Agent to Simulant Relationship Testing

Phase 1: Frame Problem

- **The application for which the simulants are needed is defined by three characteristics**

Characteristic	Example
Capability Area	**Collective Protection**
Specific Test Application	**-Swatch, Chamber, and Field Testing** **-Swatch Permeation**
Agents of Interest, and form of dissemination (defining the threat)	**GD and HD, Vapor and Liquid form**

- **Input from users and technical experts is critical to defining the problem**

Phase 2: Evaluation Model

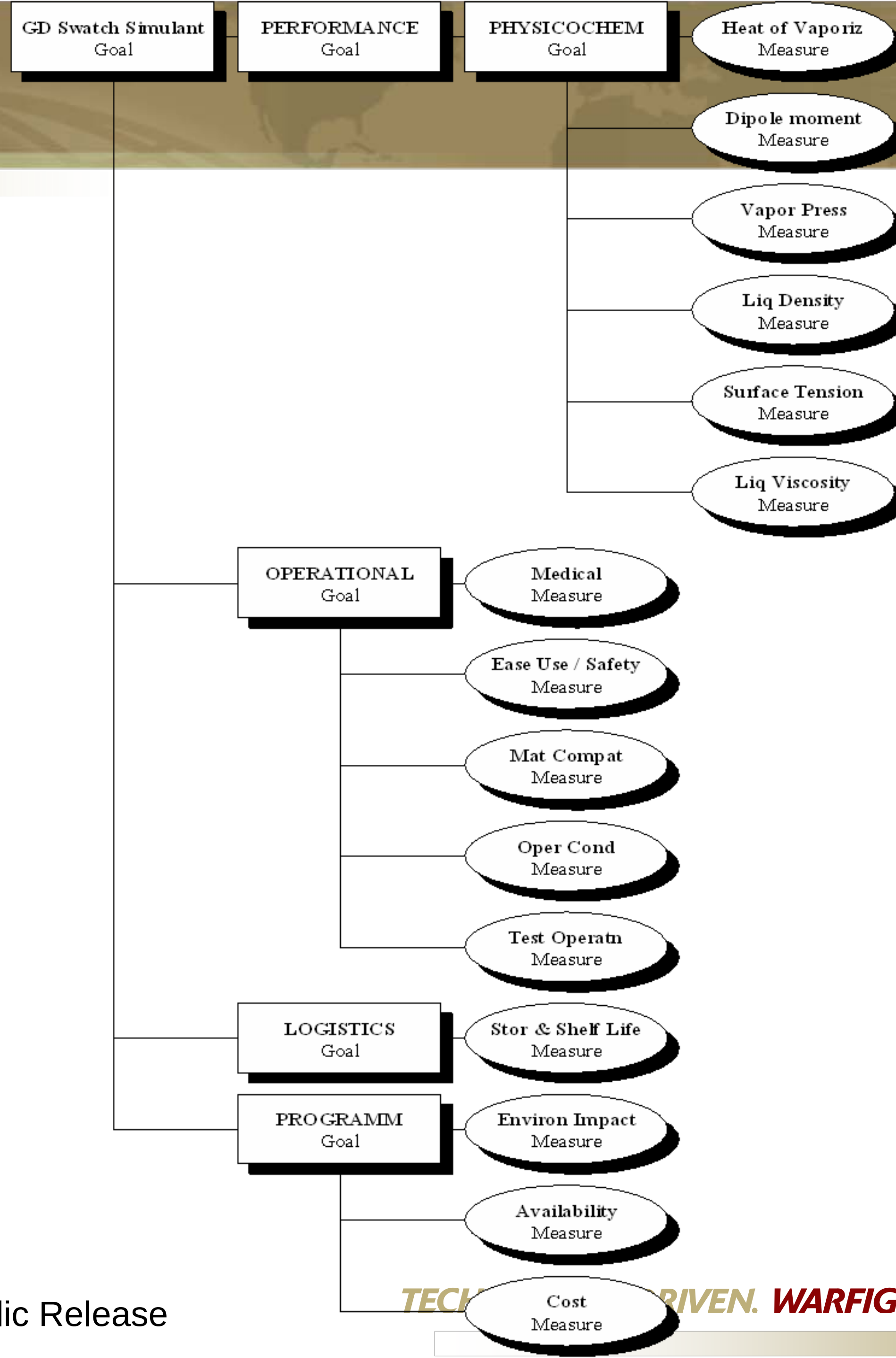
- **Model based on Multi-Attribute Utility Theory (MAUT)**
  - Decision analysis methodology for systematically evaluating alternatives/options
- **MAUT model consists of evaluation criteria, referred to as goals and measures**
  - Model typically structured as a hierarchy
  - Each goal is composed of a group of measures
  - Measures must be independent, relevant, discriminatory
- **Each measure has a definition**
- **Each measure has a performance scale**
- **Each goal/measure is weighted by importance relative to other goals/measures**

Phase 2: Evaluation Model Components

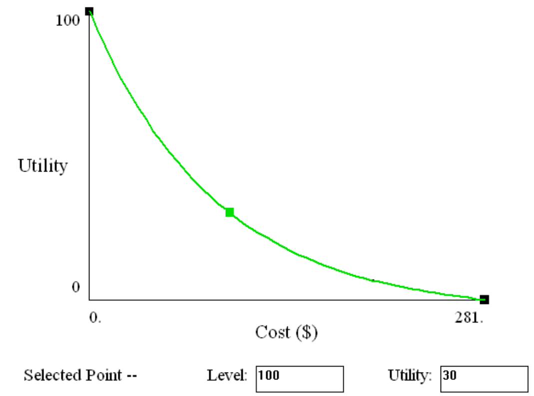
- **Model includes measures to address relevant physical and chemical properties**
  - Designed to determine the best match to the agent, to ensure that the simulant performance can be correlated to agent performance
  - Properties selected based on importance/relevance to the type of testing
- **Model also includes measures which address feasibility and practicality of use of simulant**
- **Measures weighted based on relative importance and range of chemicals being considered**
- **Three separate models developed for each agent:**
  - Swatch, chamber, and field
  - Primary model differences reflected in measure weights

Phase 2: Example Evaluation Model

(Goals and Measures)



Phase 2: Example Performance Scales

Measure	Definition	Performance Scale/Utility Curve
Cost	**Cost of obtaining sufficient quantity of the simulant for the test application under consideration**	
Environmental Impact	**Effect of the simulant on flora, fauna, and microbial systems. Simulant should not persist in the environment after test, or destroy stratospheric ozone. This work is an estimate, based on the MSDS; the final decision comes from the NEPA assessment.**	**100 – Expect no impact on environment** **50 – Expect some impact** **25 – Expect considerable impact** **0 – Expect severe impact, cannot be released, or does not degrade**

Phase 2: Example Model Weights

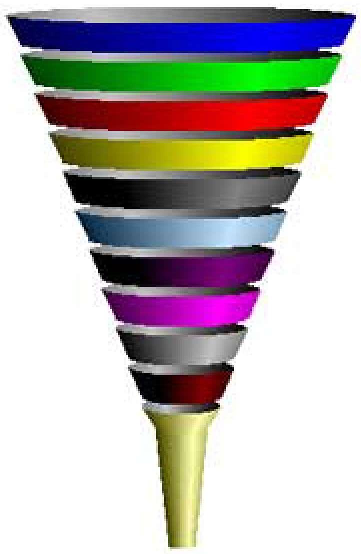
Measure	Swatch Weight	Chamber Weight	Field Weight
Physicochemical – Heat of vaporization	20	14	4
Physicochemical – Molecular Dipole	20	14	4
Physicochemical – Vapor pressure	24	17	5
Physicochemical – Liquid Density	0	0	0
Physicochemical – Surface tension	6	4	1
Physicochemical – Viscosity	8	6	1
Medical	2	3	12
Environmental impact	0	0	12
Ease of Use/Safety	1	4	7
Cost	2	4	10
Availability	2	4	6
Material Compatibility	6	12	14
Storage and Shelf Life	3	6	6
Operating Conditions	2	4	8
Test Operations	4	8	10
Total:	100	100	100

Phase 3: Identify Potential Simulants

- **Purpose is to nominate all chemicals that could be potential simulants**
- **Information Sources used:**
  - Chemical Databases (Agent/Simulant Knowledgebase [ASK], Beilstein)
  - Previous test programs (legacy simulants)
  - Research literature, published and unpublished
  - Subject Matter Expert knowledge
- **Initial data collection performed to prepare for initial screening (phase 4)**

Phase 4: Conduct Screening

- **Purpose is to use minimum threshold requirements (i.e., screening criteria) to reduce the initial list of candidate simulants**
  - Hundreds of thousands of eligible compounds
- **Screening criteria examples:**
  - Physical properties
  - Availability
  - Cost
  - Melting point
  - Boiling point
  - No stench
  - CAS number



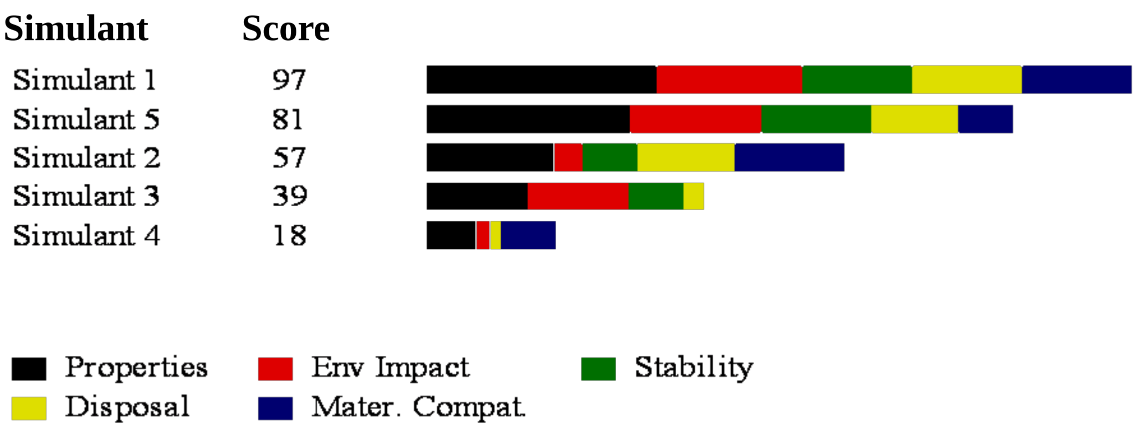
Phase 5: Collect Data

- **Perform literature search to identify and document all available information for chemicals that passed initial screen**
- **Includes verification of data/sources when feasible**
  - Data verification included identifying the temperature at which the data was collected, and recalculating if necessary to ensure that simulant and agent data points were at the same temperature
- **Sources used for initial downselects:**
  - Agent/Simulant Knowledgebase (ASK)
  - Beilstein

	Dipole moment	Heat of Vaporiz	Medical (NFPA Health rating)	Environ Impact	Ease Use/ Safety (NFPA flammability + reactivity ratings)
Simulant 1	0.55	14.7	1	20	7
Simulant 2	0.04	5.6	3	90	1
Simulant 3	0.18	9.4	2	70	4

Phase 6: Perform Evaluation and Analysis

- **Each simulant scored against each measure**
- **Linear additive method (score x weight, summed across all measures) used to generate overall score for each simulant**
- **Various analyses (sensitivity analysis) and other factors (e.g. classes of chemical) used to identify a short list of simulants to recommend for testing**



Phase 7: ASR Testing

- **Two testing steps conducted at DPG:**
  - Usability tests done to ensure feasibility of the simulant for use
  - Side-by-side comparison testing to define the specific relationship between the agent and the simulant

Initial Application: GD and HD

- **First downselect assessed and recommended simulants for HD and GD**
- **Evaluation models were the same for both agents**
- **Different lists of candidate simulants, based on matching of physicochemical properties**
  - 24 chemicals evaluated for GD, 29 for HD

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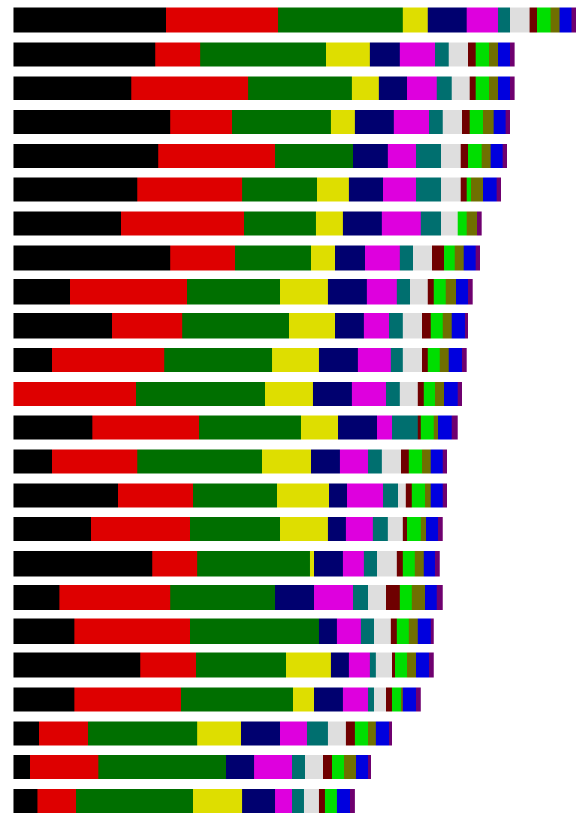
GD Simulant Scores

- *Scores for physicochemical factors based on property data gathered in phase 5*
- *Scores for non-physicochemical factors derived from other sources (such as NFPA ratings or MSDS sheets), or generated by consensus of Subject Matter Experts*
- *Rationale for scores also documented*

			GD - Physicochemical - GD						Medical	Environmental		Ease of	Cost	Availability	Material	Storage	Operating	Test
	Chemical	CAS #	Heat of vaporization	Molecular Dipole	Vapor pressure	Liquid Density	Surface tension	Viscosity	Swatch + Chamber	Swatch + Chamber	Field	Use /Safety			Compatibility	and Shelf Life	GD	Operations
GD	1,2,4-TRICHLOROBENZENE	000120-82-1	95.88	35.00	89.11	69.85	52.43	17.5	2	100	50	1	0.07	100	75	100	75	60
GD	2,6,8-Trimethyl-4-nonanone	000123-18-2; 001331-50-6	97.16	84.80	29.93	79.50	99.27	29.95	0	100	100	0	4.06	100	100	100	100	60
GD	2-Butoxyethanol; ethylene glycol monobutyl ether; butyl cellosolve	000111-76-2	99.59	57.78	45.5	87.69	92.28	99.46	2	100	75	2	0.29	100	50	50	50	60
GD	2-Ethylhexyl acetate	000103-09-3	92.17	50.00	66.08	85.04	89.51	41.2	0	100	100	2	0.02	85	75	100	75	60
GD	2-Octanol; capryl alcohol	000123-96-6	94.75	46.67	68.26	79.78	93.09	48.8	1	100	50	2	3.87	100	100	100	85	60
GD	4-CHLOROBUTYL ACETATE	006962-92-1	92.00	79.20	92.82	95.80	76.23	0.00	1	100	75	2	0.04	100	90	100	75	100
GD	4-Hydroxy-4-methyl-2-pentanone;	000123-42-2	94.39	90.00	24.71	91.04	79.03	79.66	2	100	75	2	0.02	100	100	90	85	60
GD	Aminobenzene; aniline	000062-53-3	98.92	36.94	81.84	99.49	58.17	85.36	3	100	25	2	0.06	100	50	85	75	25
GD	Benzonitrile; Cyanobenzene; Phenyl	000100-47-0	94.70	87.38	52.21	97.90	63.16	39.47	2	100	50	3	0.13	100	50	85	75	60
GD	Butyl isovalerate; Butyl 3-	000109-19-3	98.11	28.24	91.14	90.65	92.63	71.14	1	100	100	2	0.03	100	75	100	75	60
GD	Diamyl sulfide; Pentyl sulfide	000872-10-6	89.08	44.17	28.93	81.69	88.77	49.12	2	100	75	1	5.76	100	100	100		90
GD	DIETHYL ETHYLPHOSPHONATE;	000078-38-6	88.86	81.94	18.05	99.89	85.43	52.74	2	100	50	1	0.18	50	90	100	90	100
GD	Diethylene glycol monomethyl ether	000111-77-3	93.59	76.39	62.34	99.46	70.40	91.01	2	100	75	2	0.01	100	50	80	50	60
GD	DIISOPROPYL FLUOROPHOSPHATE;	000055-91-4	85.81	62.08	49.51	96.70	98.71	45.33	4	100	0	2	280.5	75	100	85	95	85
GD	DIMETHYL HEXANEDIOATE; Dimethyl	000627-93-0	80.03	66.67	15.06	96.61	70.79	78.94	1	100	75	1	0.09	100	75	100	75	60
GD	DIMETHYL HYDROGEN PHOSPHITE	000868-85-9	71.52	81.67	40.10	85.54	67.31	39.79	2	100	25	2	0.07	75	75	65	25	25
GD	Divinyl sulfone; Bis(ethenyl)sulfone	000077-77-0	97.75	81.63	51.15	86.85	79.57	75.00	3	100	25	0	4.33	100	100	0	50	100
GD	Ethyl acetoacetate	000141-97-9	94.35	90.3	48.9	99.91	76.8	49.58	2	100	100	2	0.13	100	75	100	75	60
GD	Formamide; Carbamaldehyde	000075-12-7	85.00	96.51	15.21	90.54	41.99	98.05	2	100	75	1	0.01	100	85	80	25	50
GD	Hexamethylphosphorous triamide	001608-26-0	90.39	37.78	16.71	99.79	72.27	98.38	1	100	75	3	4.74	100	100	100	75	80
GD	Methyl benzoate	000093-58-3	99.39	52.78	91.56	94.31	65.86	58.45	1	100	100	2	9.74	100	75	100	75	55

GD Example Analysis Output Swatch Permeation

Chemical	Score
Triethyl phosphate (ECBC); TEP	88
Butyl isovalerate; Butyl 3-methylbutanoate	78
Ethyl acetoacetate	78
2-Octanol; capryl alcohol	77
4-CHLOROBUTYL ACETATE	77
DIETHYL ETHYLPHOSPHONATE; DEEP	76
DIISOPROPYL FLUOROPHOSPHATE; DFP	73
2-Ethylhexyl acetate	73
4-Hydroxy-4-methyl-2-pentanone; diacetone alcohol	72
Methyl benzoate	71
TRIPROPYL PHOSPHATE; TPP	71
TRIBUTYL PHOSPHATE; TBP	70
Divinyl sulfone; Bis(ethenyl)sulfone	69
DIMETHYL HEXANEDIOATE; Dimethyl adipate	68
2-Butoxyethanol; ethylene glycol monobutyl ether; butyl cellosolve	68
Diethylene glycol monomethyl ether	67
1,2,4-TRICHLOROBENZENE	67
2,6,8-Trimethyl-4-nonanone	67
Benzonitrile; Cyanobenzene; Phenyl cyanide	66
Aminobenzene; aniline	66
DIMETHYL HYDROGEN PHOSPHITE (ECBC); DMHP	64
Hexamethylphosphorous triamide (HMPTA)	59
Triethoxymethane; TEF; triethyl orthoformate	56
Formamide; Carbamaldehyde	54



Results and Lessons Learned

- **Analysis provided information for DPG testers to select specific GD and HD simulants for usability testing**
- **Lessons learned incorporated into second downselect for GB and VX simulants:**
  - Additional sources used to identify candidate simulants, and data validation conducted concurrent with data gathering
  - Additional screening to reduce the number of chemicals for detailed evaluation
  - Evaluation model improved
    - Non-discriminating measures deleted, other key properties added
    - Criteria weights adjusted to better reflect the range of simulant scores

Future Plans

- **Use process in FY08 to support Joint Expeditionary Collective Protection (JECP) testing**
- **Continue improvements being made to process and data quality**
- **Implement process as the standard for simulant selection**
  - Can be tailored to any application, chemical or biological, that requires simulants

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